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DOCUMENTATION OF "PHOTO": A USER'S MANUAL FOR THE ANALYSIS OF PHOTOGRAPHIC AND X-RAY NEGATIVES

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This technical report has been reviewed and is approved for publication.

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This report describes the use of the program "PHOTO" in the analysis of photographic and x-ray negatives. The current capabilities and limitations of this software is described. The operational options and procedures are explained through text and examples.

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PREFACE

This report was prepared at Wright-Patterson Air Force Base by Dr. David P. Anderson. From June through September 1983 the author was employed by Universal Energy Systems, 4401 Dayton-Xenia Rd., Dayton, Ohio 45432 as a Visiting Scientist on contract number F33615-82-C-5001/SB 5448-82-C-0076. From October 1983 through August 1984 the author was employed by the University of Dayton Research Institute, 300 College Park Dr., Dayton, Ohio, on contract number F33615-81-C-5019. The USAF technical contact was Dr. W. Wade Adams, Polymer Branch, Materials Laboratory Wright Aeronautical Laboratories, AFWAL/MLBP, Wright-Patterson AFB, Ohio 45433.

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I. INTRODUCTION

This report describes the operation of the currently used, Fortran-IV, x-ray photographic analysis program, PHOTO. The previous reports (ref. 1-3) were issued by the original programmer of the software and were designed for general use. This manual describes the use of a specifically modified version of the original programs in use by the Polymer Morphology group of AFWAL/MLBP. The procedures and examples given here are typical of the type used by this group.

The program assumes that the optical densities (ranging from 0 to 3) from the negative have been digitized as eight bit binary integers. The pixel size is assumed to be 0.1mm x 0.1mm.

HARDWARE REQUIRED:

Optronics PHOTOSCAN P-1000 microdensitometer with magnetic tape,
PRIME 850 Computer including 9-track tape drive,
Tektronix 4014-1 Graphics Terminal or equivalent,
Calcomp Plotter.

SOFTWARE REQUIRED:

PRIME Operating System 19.2 or later,
Program: PHOTO,
Program: FIXDAT,
Program: MAG183.

The main steps to this procedure are:

1) Digitizing the negative and writing the information on magnetic tape for reading into the PRIME.
2) Reading the data into a disk file using the MAG183 program and ensuring the data integrity with program FIXDAT.
3) Analysis of the negative using program PHOTO.
4) Spooling plot files to the Calcomp plotter and cleaning up the directory files.

The steps described in the following sections assume the user has a basic familiarity with the computer facilities in Bldg 652.

II. OPERATIONS

1. DIGITIZING THE NEGATIVE

The basic operation of the Optronics microdensitometer is described elsewhere (ref. 4) but there are several details that need mentioning here. Since the Optronics magnetic tape system no longer writes an "End of File" message when it finishes digitizing a negative, getting the PRIME to read the tapes is tricky. The latest MAGNET tape reading utility program cannot be used. After digitizing a negative at the desired settings, you should change the record size and generate a short dummy data set. The short set must be read as a dummy file before going to the next data set. If several negatives of different sizes are to be digitized, a dummy file may not be necessary as long as each set on the tape is followed by another set with a different record size.

The tape used for data collection should ideally be cleaned, stripped, and degaussed. Blackwatch brand tapes should be avoided as the magnetic tape drive unit is not adjusted to this type. They can be identified by their shiny surface. Generally the tapes are reused several times between cleanings. The data consists of a series of records of binary numbers making up the optical densities of the negative. NRECS or NRECX is the number of records (<1000) in the file from the negative and constitutes the abscissa while NLEN or LENGTHY is the number of points (<1000) in each record and constitutes the ordinate. Since each pixel is 0.1mm x 0.1mm, the largest negative which can be examined in the program is 100mm x 100mm, but a larger negative can be analyzed piecemeal from a larger data file.

2. DATA INPUT

Once the negative(s) has been digitized, the magnetic tape is submitted to the PRIME operator for mounting on the tape drive. The Optronics microdensitomer records at a density of 800 BPI.

When logged in at any terminal, attach the appropriate user file directory (UFD) and assign the magnetic tape drive to that UFD as shown below:

OK, ATTACH ADAMS > X-RAY
OK, ASSIGN MT0
OK, RUN MAG183

(the underlined words in this manual indicate the user input)

As abbreviated version of the above is:

OK, XR
OK, AS MT0
OK, R MAG183

The user can then run the MAG183 program to read in the data from the magnetic tape. An example of this is shown in Appendix A. The required answers to program MAG183's questions are explained below:

OPTION: R (or READ) reads the tape,
MTU # = 0 this number must agree with the assigned MT#,
MT FILE # = 0 (or 1) 0 will cause the program to read the current file, while a 1 will return to the first file,
LOGICAL RECORD SIZE = lengthy LENGTHY is the record length,
BLOCKING FACTOR = 1 always 1 (records per block),
ACSII, BCD, BINARY, or EBDIC? BINARY type of numbers on file,
OUTPUT FILE: filename desired name of the data storage file. When "filename" already exists more questions are asked:
OK TO MODIFY OLD filename? Y(es) or N(o)
NO will cause the program to ask again for an OUTPUT FILE,
YES will go on:
OVERWRITE OR APPEND: O or A
O replaces the current contents of "filename" with your data,
A adds the data being read in to the end of "filename".

Since the exact value of LENGTHY may not be known, you can run MAG183 using any value the first time which will produce an

error message including the correct value of LENGTHY. For several files on the tape, each time there is a difference between the input PHYSICAL RECORD SIZE (PR) and the correct value (# READ) a similar message will be produced:

```
PHYSICAL RECORD SIZE DISCREPANCY:
SPECIFIED PR SIZE = 00, # READ = 00 AT RECORD 00 (CSW=000304)
```

For the first file you need only rerun MAG183 using MT FILE # = 1 and using the correct value of LENGTHY. For all subsequent files use "# READ=" for LENGTHY and MT FILE # = 0.

If many errors are encountered during the course of reading in the files from the magnetic tape, the user should request that the operator clean the tape drive heads. If many errors are still present when you try to reread the tape then that tape should be cleaned and the data rerecorded. A time delay of 5 minutes is not unusual if no errors are found.

After the last data file has been transferred into a disk file, the tape should be rewound, the tape drive unassigned, and the operator informed that you are finished:

```
OK, REWIND
OK, UN MTO
OK, MESSAGE
ALL FINISHED WITH THE TAPE DRIVE.
OK,
```

3. ENSURING DATA INTEGRITY

Many errors can occur during the data transfer step from magnetic tape. Two types of error messages may be printed during MAG183 operation:

```
MT ERROR, MTU=0,CSW=122304, REC#      00, UNRECOVERED
MT ERROR, MTU=0,CSW=122304, REC#      00, RECOVERED
```

If any of these or other errors are present the data file should be corrected with FIXDAT. The recovered errors are not as

serious as the unrecovered errors since this usually means the record was eventually read. Other errors are possible which do not generate any error message.

A distortion of 0.1mm is created for each data record not successfully read (unrecovered error) or partially duplicated (recovered error). The FIXDAT program reads the record numbers, contained in the first four words of the record, and detects missing and duplicate records. Only the last duplicate record (the one without errors) is kept while all others are deleted. Missing records are replaced with the proceeding record. These corrections maintain distances between features with minimal intensity distortion.

The program FIXDAT will ask for the filename (data file form MAG183), output filename, the number of records and record length. It will also ask for the number of lines and records to be skipped, but these last are usually zero. Appendix A includes an example of this operation. At the end of the program execution, a summary of the number or records added, subtracted, and total on the negative is printed.

If LENGTHY is set to 4, the program will determine whether the file needs correcting. This saves time only if corrections are not necessary. This should be done only if no MT errors were encountered when reading in the file but other errors are suspected by the user.

4. PATTERN ANALYSIS

The program PHOTO does the actual analysis of negatives. It is an interactive program which can do the following:

-Open and close files used by the program.

-Read the binary optical density file and convert it into decimal numbers and/or related intensities.

-Produce contour plots on a Tektronix terminal, AED color terminal, or off-line on a Calcomp plotter.

-Enlarge part of the contour plot or create a subplot of a peak.

-Locate a specific point or the position of a peak from the contour.

-Find the center position of several peaks, points, or rings.

-Generate plots of optical density or relative intensity versus distance from a point at any angle, or versus angle at any distance from a point.

-Convert film position to diffraction angle or reciprocal space vector.

-The data from any scan can be saved on a data file for further analysis, such as curve fitting, by other programs.

This program is executed in UFD ADAMS X-RAY by typing:

OK, SEG #PHOTO

A sample session is shown in Appendix B but all options are described below (you may type just a "Return" for any question with a default answer):

ENTER DATA FILE NAME

This file, located in the current UFD, contains the binary optical density values read in from magnetic tape. The filename may contain up to 32 characters.

ENTER RUN IDENT (12 CHAR MAX)

This is the run identification, the 12 characters are printed on the various plots generated by the program. This identity is also prefixed by P. and S. as names of the off-line plot file and data save file respectively.

a. Read Data Section

ENTER NRECX, LENGTHY, NSKIPX, NSKIPY

NRECX is the number of records as determined during the MAG183 read in of data. NLENGTHY is the length of each record on the negative's file. NSKIPY is the number of records the user desires to skip on the right hand side of the negative. NSKIPY

is the number of data points skipped in each record, taken from the top of the negative. There is generally a several minute wait after typing in these parameters during which the data is transferred into the work space.

b. Contour Section

DO YOU WANT TO GO TO THE CONTOUR SECTION? Y/N

Allows you to perform all contour options as explained below if you enter the CONTOUR section. "Y" is the default, "N" sends you to the same point in the main program as when you exit this section.

DO YOU WANT A PLOT? Y/N

This option produces a contour plot of the negative and allows you to use one of several contour options below. "Y" is the default and produces:

WANT TO CHANGE CONTOUR LEVELS? Y/N

A "Y" response will cause the current levels to be printed and then ask for 8 new levels. The default (N) contour levels are:

0.50, 0.75, 1.00, 1.25, 1.50, 1.75, 2.00, and 2.50.

After changing the levels or accepting the current ones, the program calculates an array containing up to 150 x 150 elements by averaging the optical densities in an MxM square box of pixels. The program automatically calculates M so that either x or y has 150 elements, whichever direction is longest. There is a several minute delay for these calculations. The program pauses at the end of the plot to allow the user to get a Tektronix hard copy if that is desired. This program pauses at the end of all on-line plots.

At the end of the contour plot, typing any character and hitting the "return" causes the program to list the options and ask which option is desired:

OPTIONS ARE:

1. RETURN TO MAIN PROGRAM
2. OFFLINE CALCOMP PLOT
3. AED COLOR PLOT
4. RESET TO ON-LINE PLOT
5. FIND PEAK MAX POSITION
6. FIND CURSOR COORDINATES
7. FIND RINGS CENTER
8. REDRAW CONTOURS
9. CHANGE PLOT FACTOR
10. BLOW-UP PART OF PLOT
11. CREATE SUBPLOT
12. PEAK VOLUME
13. MOVIE, BYU PREPARATION
14. LINE AVERAGE SLICE PLOT

ENTER OPTION NUMBER:

Typing a number less than 1 or greater than 14 will produce an error message followed by the same list. The purpose and results of each option is listed below. Any needed information is requested by the option in a self-explanatory fashion.

1 - Returns to the main program as described below.

2 - Transfers the information from the last contour plot onto the Calcomp plot file.

3 - Prepares color contour plots if the user is on an AED color terminal.

4 - Resets the program to accept data, such as cursor coordinates, from the current on-line plot. This needs to be done for the following options: 5, 6, 7, 10, 11, 12, 14.

5 - Searches a 4mm square for a peak maximum. The position of the center of this box is set by positioning the cursors and typing any character, except "X" which terminates the search for peaks. Up to 40 peaks may be located each time you enter this option. Pairs of peaks can be used to determine the center of the plot, see Appendix B. This will set the I0 and J0 variables when returning to the main program.

6 - Locates the cursor coordinates when positioned and a character is entered. An "X" will also terminate this option. The center of all positions can also be used to set I0 and J0.

7 - Asks the user to set the approximate center of the rings with the cursors (enter any character after positioning). Two different angles are requested which are scanned for maxima, the position and optical density of each maximum are listed and the user must match the appropriate pairs (at least one). The program then geometrically calculates the true center of the rings. (see Appendix B)

8 - Causes the contour plot to be regenerated on the terminal screen.

9 - Changes the scaling factor for a replot of the contours.

10 - Allows you to zoom in on a small section of the contour plot.

11 - Generates a subplot file of any peak for off-line plotting. (filename = SP. indent).

12 - Calculates the volume under a peak.

13 - Prepares several files for use with the Brigham Young University "MOVIE" program.

14 - Plots an optical density versus position scan that uses average ODs from a line perpendicular to the scan.

Option 1 terminates the CONTOUR section and returns the operation to the main program.

c. Plot Position and Condition Section

On returning to the main program, the origin for the remaining scans, I0 and J0, will be printed if they have been set and the program will ask if the user wants them changed. If either I0 or J0 is greater than the maximum allowed or less than or equal to 0, then an error message will be printed and new values requested.

```
I0= OOO,  J0 = OOO
DO YOU WISH TO CHANGE I0 OR J0?  Y/N
Other questions asked are:
DO YOU WANT THE DATA SMOOTHED?  Y/N
```

"Y" (default) involves smoothing the scans below with a 9 point smoothing routine.

DO YOU WANT RELATIVE INTENSITIES? Y/N

A "Y" will cause some questions involving which type of film and radiation were used so that relative intensities can be calculated from the optical densities.

WHAT FILM TYPE DID YOU USE AGFA/AA/DEF-5
WHAT TYPE OF RADIATION WAS USED? CU/FE/MO

Each questions needs the first two letters of the appropriate answer. Effective July 1, 1984 the program was calibrated for the following film and radiation types, but more will be added later.

Osray AGFA film for Cu, Mo, and Fe radiation,
Kodak AA film for Cu and Mo radiation,
Kodak DEF-5 film for Cu radiation.

"N" (default) merely continues to the next question.

IS THIS A GUINIER PLOT? Y/N
DO YOU WANT THE DISTANCES COVERTED TO AN ANGULAR MEASUREMENT? Y/N

This option applies only to flat film x-ray negatives. "N" (default) proceeds with the program, but "Y" will cause the program to ask:

DO YOU WANT PLOTS WITH TWO THETA (T) OR RECIPROCAL SPACE VECTOR (S) VALUES?
WHAT IS THE SAMPLE TO FILM DISTANCE (CM)?
WHAT WAVELENGTH X-RAYS DID YOU USE (ANGSTROMS)?
(CU-K-ALPHA = 1.5418)

The last question is for the "S" option only. The "T" or "S" option will change the standard scales for radial plots below to +/-60 DEGREES or +/-0.6 1/A respectively.

In the next question the user decides who will scale the plots.

DO YOU WANT THE AXES SCALED BY THE PROGRAM? Y/N/S

S=STANDARD: +/- 40MM (RADIAL) OR,

S=STANDARD: 0 TO 180 DEGREES (PSI).

The "standard" axes are listed in the question for the x-axis with the y-axis being set to 0-3 for optical density or 0-1.2 for relative intensity This option is useful if you wish to examine several scans quickly.

The program will automatically scale the plots to fill most of available areas with the "Y" option. An "N" will cause the program, just prior to the plot, to list the minimum and maximum values of x and y and ask for the desired minimum axis values and the incremental values per inch.

Both "S" and "N" options may involve truncation of part of the plot which may be desired in order to see the detail in a region of interest or to cut out unwanted noise.

d. Guinier Plot Section

If the negative was taken on Guinier camera a "Y"to the Guinier plot question will cause the program to calculate diffraction angles assuming the film radius is 57mm and set several other parameters. The rest of a Guinier scan is the same as a radial plot (see Section e, Radial Scan) from the "ANGLE TO X-AXIS" question below.

e. Radial Scan Section

The RADIAL section scan section begins by asking:

DO YOU WANT A RADIAL SCAN? Y/N

This section will calculate the intensity along a line through I0 and J0 at an angle, PSI, to the x-axis of the contour plot.

ENTER SCAN ANGLE TO X-AXIS (DEGREES);

You may choose any PSI angle between 0 and 180 degrees. The negative scan positions will always be in the second or third

quadrant. If you chose the manual scaling, then the program will ask for the appropriate initial and incremental values, then go on:

AT THE END OF THE PLOT, TYPE "Y" TO FIND THE SEPARATION,
OTHERWISE TYPE "RETURN".

READY TO PLOT? Y/N

An "N" cancels the entire plot and puts the user at the main program OPTION section. When the plot is finished you can find the separation between points on the x-axis by typing a "Y" and then positioning the vertical cursor at any two points. Any character entered will fix one point at the current cursor position. You can continue to find the distance between any two positions by again entering a "Y". Any other input will elicit:

CALCOMP PLOT? Y/N

A "Y" will cause the Tektronix plot on the screen to be transferred to the plot file.

DO YOU WANT TO SAVE THE DATA FROM THIS SCAN? Y/N

is the next question. The data is output onto the save file as x,y pairs, using the units and values currently plotted.

DO YOU WANT ANOTHER SCAN? Y/N

A "Y" will return the user to the start of the RADIAL section, an "N" will transfer the user to the OPTION section. The OPTION section is discussed after the PSI section below.

f. Psi Section

The beginning of the PSI section includes a help option:

DO YOU NEED HELP TO DETERMINE THE RADIUS? Y/N

An "N" goes on to requesting the radius, while a "Y" requests a minimum and maximum radius (in mm) which defines an annulus in which a maximum is hunted. If a maximum is found:

LOCAL MAXIMUM AT RADIUS + 00.0mm

is printed and the program continues. If no maximum is found:

NO LOCAL MAXIMUM. RADIUS = 00.0 IS THE HIGH SIDE
DO YOU WANT TO TRY AGAIN? Y/N

A "Y" goes back to requesting the annulus limits and an "N" continues.

The program then asks:

ENTER: RADIUS (MM), PSI0, PSIF

or for the "standard" scaling option:

ENTER: Radius (MM)

The standard initial PSI angle (PSI0) is 0 and the final PSI angle (PSIF) is 180 degrees.

The plotting of intensity versus angles follows the same sequence of questions as in the RADIAL section. The one exception is that the separation of positions is given in degrees rather than millimeters

g. Option Section

The next and final section is the main program Option section which automatically occurs at the end of any scan plot section or when a plot is canceled:

OPTION CODES:
1 - RE-READ DATA
2 - CONTOUR SECTION
3 - CHANGE PLOT POSITION OR CONDITIONS
4 - GUINIER PLOT SECTION
5 - RADIAL SCAN SECTION
6 - PSI SCAN SECTION
7 - STOP

1 - Returns to near the beginning of the program to the Read Data Section.

2 - Goes back to the beginning of the Contour Section.

3 - Returns to Plot Position and Condition Section.

4 - Goes to Guinier Plot Section.

5 - Begins the Radial Scan Section.

6 - Goes to the help option of the PSI section.

7 - Will cause:

h. Stop Section

ARE YOU FINISHED? Y/N

Any response but a "Y" will return you to the start of the Option section. This question allows you a second chance to stay in the program and avoid the several minute delay required to reread the data if you haven't finished all the plots. A "Y" will terminate the program after asking the following questions:

DO YOU WANT TO KEEP THE "SAVE" FILE? Y/N
DO YOU WANT TO KEEP THE "PLOT" FILE? Y/N

Only a "Y" to these questions will retain these files that were opened at the beginning of the program. Exiting the program at any other point, however will not delete these files.

5. FINAL PROCEDURES

If you asked PHOTO to produce Calcomp plots, you must spool the plot file so that the operator can generate those plots:

OK, SPOOL P.ident -FORMS PLOT

or

OK, SPLT P.ident

The latter is simply an abbreviation in the ADAMS UFD for the former. The plot can then be obtained, usually within an hour, from building 652. If the program was not exited normally, this file may have to be closed:

OK, CLOSE ALL

or

OK, C ALL

or

OK, CLOSE P.ident

Since disk space is limited, all unneeded files should be deleted. Once a plot file is spooled it can be deleted. Save files can be listed or transferred to another UFD and then deleted. Data files particularly (both raw and "fixed") take up the most space and should be deleted when they are no longer needed.

```
OK, DELETE filename
```

or for many plot or save files

```
OK, FUTIL
 >CLEAN P.
 >CLEAN S.
 >Q
 OK,
```

The "clean" command deletes all files beginning with the characters following it, so be sure that all those files should be deleted.

REFERENCES

1. Ford, Dale L., "XRYSTEP Computer Programs to Assist in the Analysis of X-ray Crystallographic Negatives", UDR-TM-79-25, 1979.

2. Ford, Dale L., "User's Guide for the Analysis of X-ray Patterns", UDR-TM-80-24, July 1980.

3. Ford, Dale L., "User's Guide for the Analysis of Digitized Photonegatives", UDR-TM-81-07, January 1981.

4. "OPERATING INSTRUCTIONS Photoscan System P-1000", Optronics International, Inc., Chelmsford, MA 1971. (kept next to the microdensitometer)

APPENDIX A

EXAMPLE OF DATA INPUT AND INTEGRITY CHECK

Data Input:

```
OK, ASSIGN MT0
Device MT0 assigned.
OK, R MAG183

[MAGNET rev. 18.1]

OPTION: R
MTU # = 0
MT FILE # = 0
LOGICAL RECORD SIZE = 100
BLOCKING FACTOR = 1
ASCII, BCD, BINARY, OR EBCDIC? BINARY
OUTPUT FILE: TEST1

PHYSICAL RECORD SIZE DISCREPANCY:
SPECIFIED PR SIZE =   100, # READ =   648 AT RECORD          1   (CSW=000300)

RECORD SIZE ERROR
ER! R MAG183

[MAGNET rev. 18.1]

OPTION: R
MTU # = 0
MT FILE # = 1
LOGICAL RECORD SIZE = 648
BLOCKING FACTOR = 1
ASCII, BCD, BINARY, OR EBCDIC? BINARY
OUTPUT FILE: TEST1
OK TO MODIFY OLD TEST1? Y
OVERWRITE OR APPEND: O
MT ERROR, MTU=0, CSW=122300, REC#=        669, UNRECOVERED

PHYSICAL RECORD SIZE DISCREPANCY:
SPECIFIED PR SIZE =   648, # READ =   598 AT RECORD        670   (CSW=000300)

RECORD SIZE ERROR
ER! R MAG183

[MAGNET rev. 18.1]

OPTION: R
MTU # = 0
MT FILE # = 0
LOGICAL RECORD SIZE = 598
BLOCKING FACTOR = 1
ASCII, BCD, BINARY, OR EBCDIC? BINARY
OUTPUT FILE: DUMMY
MT ERROR, MTU=0, CSW=122300, REC#=         19, UNRECOVERED

PHYSICAL RECORD SIZE DISCREPANCY:
SPECIFIED PR SIZE =   598, # READ =   648 AT RECORD         20   (CSW=000300)

RECORD SIZE ERROR
```

```
ER! R MAG183

[MAGNET rev. 18.1]

OPTION: R
MTU # = 0
MT FILE # = 0
LOGICAL RECORD SIZE = 648
BLOCKING FACTOR = 1
ASCII, BCD, BINARY, OR EBCDIC? BINARY
OUTPUT FILE: TEST2
MT ERROR, MTU=0, CSW=122300, REC#=       667, UNRECOVERED
MT ERROR, MTU=0, CSW=122300, REC#=       706, UNRECOVERED
MT ERROR, MTU=0, CSW=122300, REC#=       745, UNRECOVERED

PHYSICAL RECORD SIZE DISCREPANCY:
SPECIFIED PR SIZE =   648, # READ =   598 AT RECORD       746  (CSW=000300)

RECORD SIZE ERROR
Now at command level 5. To release use RLS. (listen_)
ER! RLS
OK, REWIND
OK, UN MTO
Device released.
OK, M
ALL FINISHED WITH THE TAPE DRIVE.
OK,
*** SYSTEM at 10:17
OK



C ALL
```

Ensuring Data Integrity:

```
OK, SEG #FIXDAT
ENTER DATA FILE NAME  TEST2
ENTER OUTPUT FILE NAME  TESTFIX
ENTER  NRECX, LENGTHY, NSKIPX, NSKIPY
745 648 0 0
WARNING: AT LINE  667,   1 LINE(S) INSERTED
WARNING: AT LINE  706,   1 LINE(S) INSERTED
 END OF FILE AT LINE NO. 745
ON THIS NEGATIVE  744 LINES READ AND  753 WRITTEN
OK,
```

APPENDIX B

EXAMPLE OF PATTERN ANALYSIS

```
OK, SEG *PHOTO

 DATE: 07/06/84
 TIME: 13:17:45

 ENTER DATA FILE NAME
TEST1
 ENTER RUN IDENT (12 CHAR MAX)
EXAMPLE
 ENTER NRECX, LENGTHY, NSKIPX, NSKIPY
660 598 0 0
 DO YOU WANT TO GO TO THE CONTOUR SECTION?  Y/N
Y
 DO YOU WANT A PLOT?  Y/N                          (use "Y" default)
 WANT TO CHANGE CONTOUR LEVELS?  Y/N
Y
 PRESENT CONTOUR VALUES ARE:
 0.50 0.75 1.00 1.25 1.50 1.75 2.00 2.50
 ENTER EIGHT NEW VALUES.
0.4 0.6 0.8 1.0 1.4 1.8 2.2 2.6
 AFTER THE PLOT IS FINISHED TYPE ANY CHARACTER   NOW HIT RETURN.

              (figure 1 generated)

 OPTIONS ARE:
   1  - RETURN TO MAIN PROGRAM
   2  - OFFLINE CALCOMP PLOT
   3  - AED COLOR PLOT
   4  - RESET TO ON-LINE PLOT
   5  - FIND PEAK MAX POSITION
   6  - FIND CURSOR COORDINATES
   7  - FIND RINGS CENTER
   8  - REDRAW CONTOURS
   9  - CHANGE PLOT FACTOR
  10  - BLOW-UP PART OF PLOT
  11  - CREATE SUBPLOT
  12  - PEAK VOLUME
  13  - MOVIE.BYU PREPARATION
  14  - LINE AVERAGED SLICE PLOT

 ENTER OPTION NUMBER:  5

 NO    I     J     O D
  1   185   371   3.00
  2   220   370   2.57
  3   421   380   2.68
  4   456   377   3.00

ENTER PAIR NUMBERS: USE DUP *S TO END

 1 4
 2 3
 1 1

  PAIR  DIST.  ORIGIN   ROTATION
    1   27.11  320  374   1.27
    2   20.12  320  375   2.85

 I0 = 321  J0 = 375  ROT =  2.06

  DO YOU WISH TO TRY OTHER PAIRS?  Y/N :N
  DO YOU WANT TO CHANGE I0 & J0?  Y/N :N

 EXAMPLE
  NO    I     J     INT  RADIUS   ANGLE
   1  -136   -4   3.00   13.61    1.68
   2  -101   -5   2.57   10.11    2.83
   3   100    5   2.68   10.01    2.86
   4   135    2   3.00   13.50    0.85
```

```
 DO YOU WISH TO DO THIS OVER?  Y/N :N
 ENTER OPTION NUMBER:  7
 INPUT THE APPROXIMATE CENTER WITH THE CURSORS

 WHAT ANGLE DO YOU WANT TO SCAN FOR PEAKS?
45
 N0.     INTEN    DIST MM
  1      0.262     -39.8
  2      0.449     -27.8
  3      0.447     -26.7
  4      0.437     -23.3
  5      0.749     -15.6
  6      1.693      -9.6
  7      1.374      -3.0
  8      1.556       3.3
  9      1.843      10.4
 10      1.374      12.7
 11      0.821      16.6
 12      0.480      24.6
 13      0.505      28.3

 INPUT PEAK PAIRS FOR CENTERING BY NUMBER.
   (INPUT IDENTICAL NUMBERS AFTER LAST PAIR)
5 11
6 9
1 1

 WHAT SECOND ANGLE DO YOU WANT?
   (DIFFERENT FROM THE FIRST AND BEST IF PERPENDICULAR)
135
 N0.     INTEN    DIST MM
  1      0.462     -27.8
  2      0.436     -23.9
  3      0.768     -16.2
  4      1.783     -10.0
  5      1.867      -2.8
  6      0.228       0.5
  7      1.333       2.9
  8      1.729      10.0
  9      0.757      16.2
 10      0.450      23.6
 11      0.465      25.7
 12      0.482      27.9
 13      0.243      44.8
 14      0.245      45.9

 INPUT PEAK PAIRS FOR CENTERING BY NUMBER.
   (INPUT IDENTICAL NUMBERS AFTER LAST PAIR)
3 9
4 8
2 2

 CURRENT CENTER IS I=318 AND J=370
 THE NEW CENTER IS I=321 AND J=373
 DO YOU WANT TO TRY AGAIN?  Y/N
N
 ENTER OPTION NUMBER:  1

 I0= 321  J0= 373
 DO YOU WISH TO CHANGE I0 OR J0?  Y/N
N
 DO YOU WANT THE DATA SMOOTHED?  Y/N
Y
 DO YOU WANT RELATIVE INTENSITIES?  Y/N
N
 IS THIS A GUINIER PLOT?  Y/N
N
 DO YOU WANT THE DISTANCES CONVERTED TO AN ANGULAR
    MEASUREMENT?  Y/N
N
 DO YOU WANT THE AXES SCALED BY THE PROGRAM?  Y/N/S
   S=STANDARD:  +/- 40 MM  (RADIAL) OR,
   S=STANDARD: 0 TO 180 DEGREES  (PSI).
N
```

```
 DO YOU WANT A RADIAL SCAN?  Y/N
Y
 ENTER SCAN ANGLE TO X AXIS (DEGREES) :
2.85
 THE MIN VALUE IS -32.00   THE MAX VALUE IS  33.90
 THIS AXIS IS  8.  INCHES LONG.
 WHAT START AND INCH INCREMENT DO YOU WANT?
-40. 10
 THE MIN VALUE IS   0.13   THE MAX VALUE IS   3.17
 THIS AXIS IS  6.  INCHES LONG.
 WHAT START AND INCH INCREMENT DO YOU WANT?
0 .5
 AT THE END OF THE PLOT, TYPE "Y" TO FIND
 THE SEPARATION, OTHERWISE TYPE "RETURN".

 READY TO PLOT?  Y/N
```

(figure 2 generated)

```
 CALCOMP PLOT?  Y/N :  N
 DO YOU WANT TO SAVE THE DATA FROM THIS SCAN?  Y/N
N
 DO YOU WANT ANOTHER SCAN?  Y/N
N

 OPTION CODES:
   1 - RE-READ DATA
   2 - CONTOUR SECTION
   3 - CHANGE PLOT POSITION OR CONDITIONS
   4 - GUINIER PLOT SECTION
   5 - RADIAL SCAN SECTION
   6 - PSI SCAN SECTION
   7 - STOP
 ENTER DESIRED CODE:  3
 I0= 321  J0= 373
 DO YOU WISH TO CHANGE I0 OR J0?  Y/N
N
 DO YOU WANT THE DATA SMOOTHED?  Y/N
Y
 DO YOU WANT RELATIVE INTENSITIES?  Y/N
Y
 WHAT FILM TYPE DID YOU USE?  AGFA/AA/DEF-5
AA
 WHAT TYPE OF RADIATION WAS USED?  CU/FE/MO
CU
 IS THIS A GUINIER PLOT?  Y/N
N
 DO YOU WANT THE DISTANCES CONVERTED TO AN ANGULAR
    MEASUREMENT?  Y/N
Y
 DO YOU WANT PLOTS WITH TWO THETA (T) OR
    RECIPROCAL SPACE VECTOR (S) VALUES?
S
 WHAT IS THE SAMPLE TO FILM DISTANCE (CM)?
2.91
 WHAT WAVELENGTH X-RAYS DID YOU USE (ANGSTROMS)?
    (CU-K-ALPHA = 1.5418 A)
1.5418
 DO YOU WANT THE AXES SCALED BY THE PROGRAM?  Y/N/S
   S=STANDARD:  +/- 0.6  1/A  (RADIAL) OR,
   S=STANDARD: 0 TO 180 DEGREES  (PSI).
N

 DO YOU WANT A RADIAL SCAN?  Y/N
Y
 ENTER SCAN ANGLE TO X AXIS (DEGREES) :
92.85
 THE MIN VALUE IS  -0.41   THE MAX VALUE IS   0.57
 THIS AXIS IS  8.  INCHES LONG.
 WHAT START AND INCH INCREMENT DO YOU WANT?
-0.6 0.15
 AT THE END OF THE PLOT, TYPE "Y" TO FIND
 THE SEPARATION, OTHERWISE TYPE "RETURN".
```

```
 READY TO PLOT?  Y/N
Y
                (figure 3 generated)

 CALCOMP PLOT?  Y/N :  Y
 DO YOU WANT TO SAVE THE DATA FROM THIS SCAN?  Y/N
Y
 THE FITTING PROGRAM ASSUMES TWO-THETA POSITIONS
 DO YOU WANT ANOTHER SCAN?  Y/N
N
 OPTION CODES:
    1 - RE-READ DATA
    2 - CONTOUR SECTION
    3 - CHANGE PLOT POSITION OR CONDITIONS
    4 - GUINIER PLOT SECTION
    5 - RADIAL SCAN SECTION
    6 - PSI SCAN SECTION
    7 - STOP
 ENTER DESIRED CODE:  3

 I0= 321  J0= 373
 DO YOU WISH TO CHANGE I0 OR J0?  Y/N
N
 DO YOU WANT THE DATA SMOOTHED?  Y/N
Y
 DO YOU WANT RELATIVE INTENSITIES?  Y/N
N
 IS THIS A GUINIER PLOT?  Y/N
N
 DO YOU WANT THE DISTANCES CONVERTED TO AN ANGULAR
     MEASUREMENT?  Y/N
N
 DO YOU WANT THE AXES SCALED BY THE PROGRAM?  Y/N/S
    S=STANDARD:  +/- 40 MM  (RADIAL) OR,
    S=STANDARD: 0 TO 180 DEGREES  (PSI).
N
 DO YOU WANT A RADIAL SCAN?  Y/N
N
 DO YOU WANT TO SCAN IN THE PSI DIRECTION?  Y/N
Y
 DO YOU NEED HELP TO DETERMINE RADIUS?  Y/N
Y
 ENTER MIN AND MAX RADIUS (MM):
9.9 10.3
 LOCAL MAXIMUM AT RADIUS=   10.1 MM
 ENTER:  RADIUS (MM), PSI0, PSIF
10.1 0 360
 THE MIN VALUE IS    0.00   THE MAX VALUE IS 360.00
 THIS AXIS IS  8.  INCHES LONG.
 WHAT START AND INCH INCREMENT DO YOU WANT?
0 45
 THE MIN VALUE IS   1.54   THE MAX VALUE IS   2.71
 THIS AXIS IS  6.  INCHES LONG.
 WHAT START AND INCH INCREMENT DO YOU WANT?
0 .5

 AT THE END OF THE PLOT, TYPE "Y" TO FIND
 THE SEPARATION, OTHERWISE TYPE 'RETURN'.

 READY TO PLOT?  Y/N
Y
                (figure 4 generated)

 CALCOMP PLOT?  Y/N :  N
 DO YOU WANT TO SAVE THE DATA FROM THIS SCAN?  Y/N
N
 DO YOU WANT ANOTHER SCAN?  Y/N
N
 OPTION CODES:
    1 - RE-READ DATA
    2 - CONTOUR SECTION
```

```
   3 - CHANGE PLOT POSITION OR CONDITIONS
   4 - GUINIER PLOT SECTION
   5 - RADIAL SCAN SECTION
   6 - PSI SCAN SECTION
   7 - STOP
 ENTER DESIRED CODE:  7
 ARE YOU FINISHED?  Y/N
Y
DO YOU WANT TO KEEP THE "SAVE" FILE?  Y/N
Y
DO YOU WANT TO KEEP THE "PLOT" FILE?  Y/N
Y


OK,
```

Final Procedures:

```
OK, SPLT P.EXAMPLE
[SPOOL rev 19.2.3]
PRT003 spooled,  records:     1, name: P.EXAMPLE

 user   prt  time   name              size  opts/*   form   defer   at: PR0
------ --- -----  ---------------- -----  ------  ------  -----  ----------
EDDMO  001*14:51  PG01VHSIC           3          PLOT
PETERS 002*15:27  L_HOPFIT7           36
ADAMS  003 15:27  P.EXAMPLE           1          PLOT

* means file being printed.
OK, DELETE P.EXAMPLE


OK, ALIST S.EXAMPLE
**ALIST** [122578]
EXAMPLE                    RADI  TEST1                      660  598    0
    1  90.00  321  373   91
  -0.09941    0.90472
  -0.09724    0.91868
  -0.09507    0.92383
  -0.09289    0.93018
  -0.09071    0.92882
  -0.08853    0.92745
  -0.08635    0.92723
  -0.08416    0.93089
  -0.08197    0.94030
  -0.07978    0.95312
```

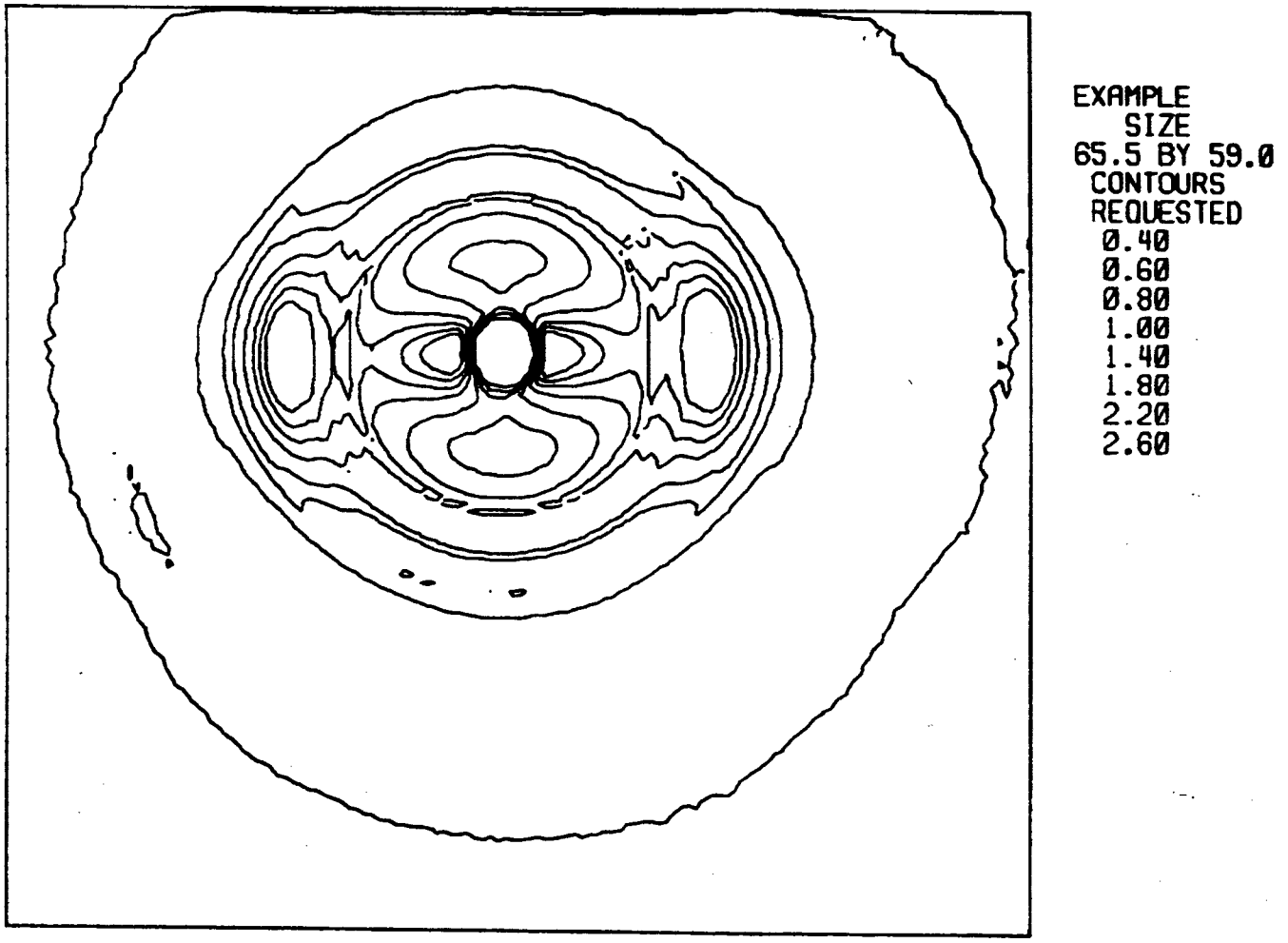

Figure 1. Contour Plot.

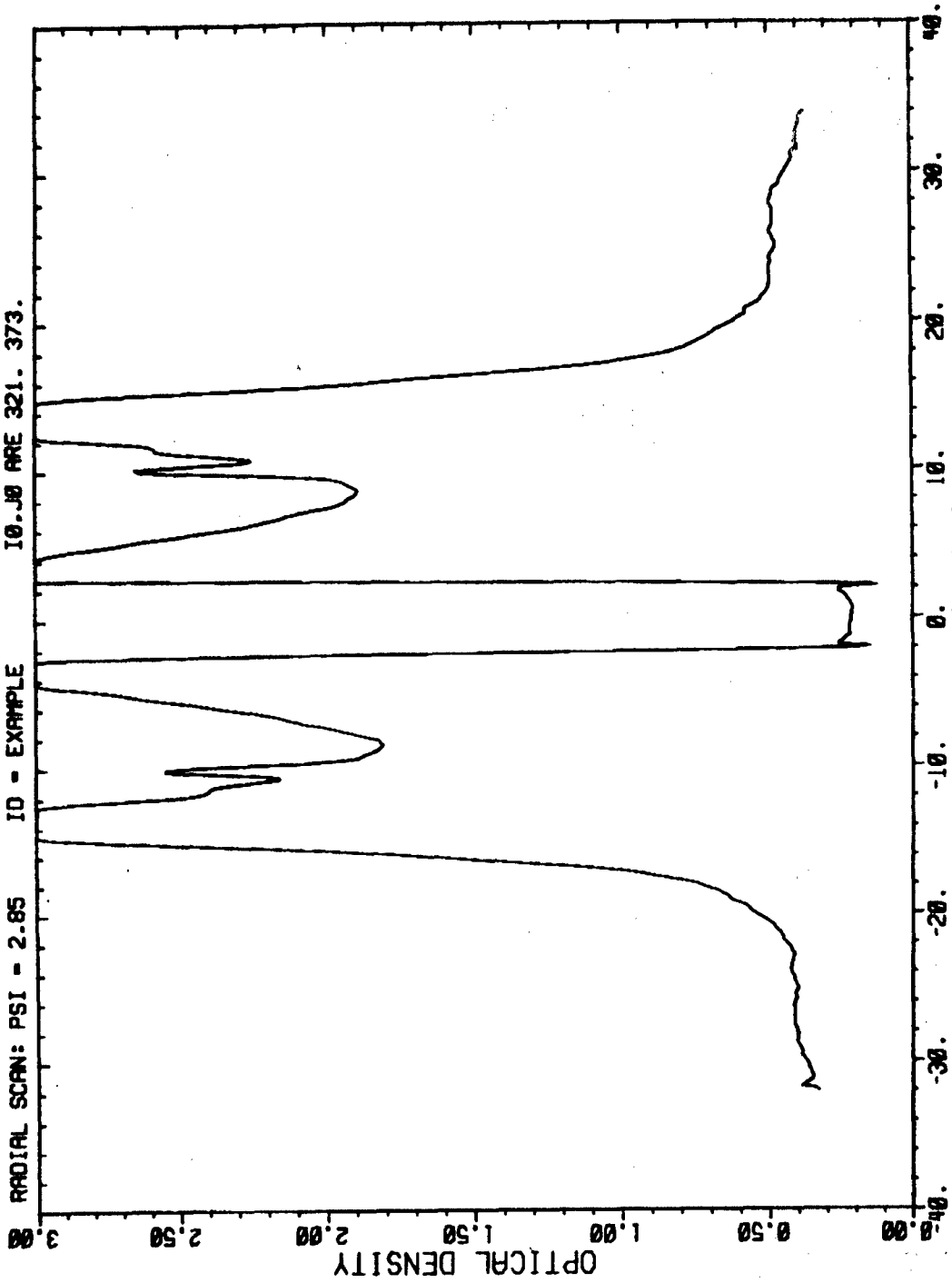

Figure 2. Radial Plot: Optical Density vs Position.

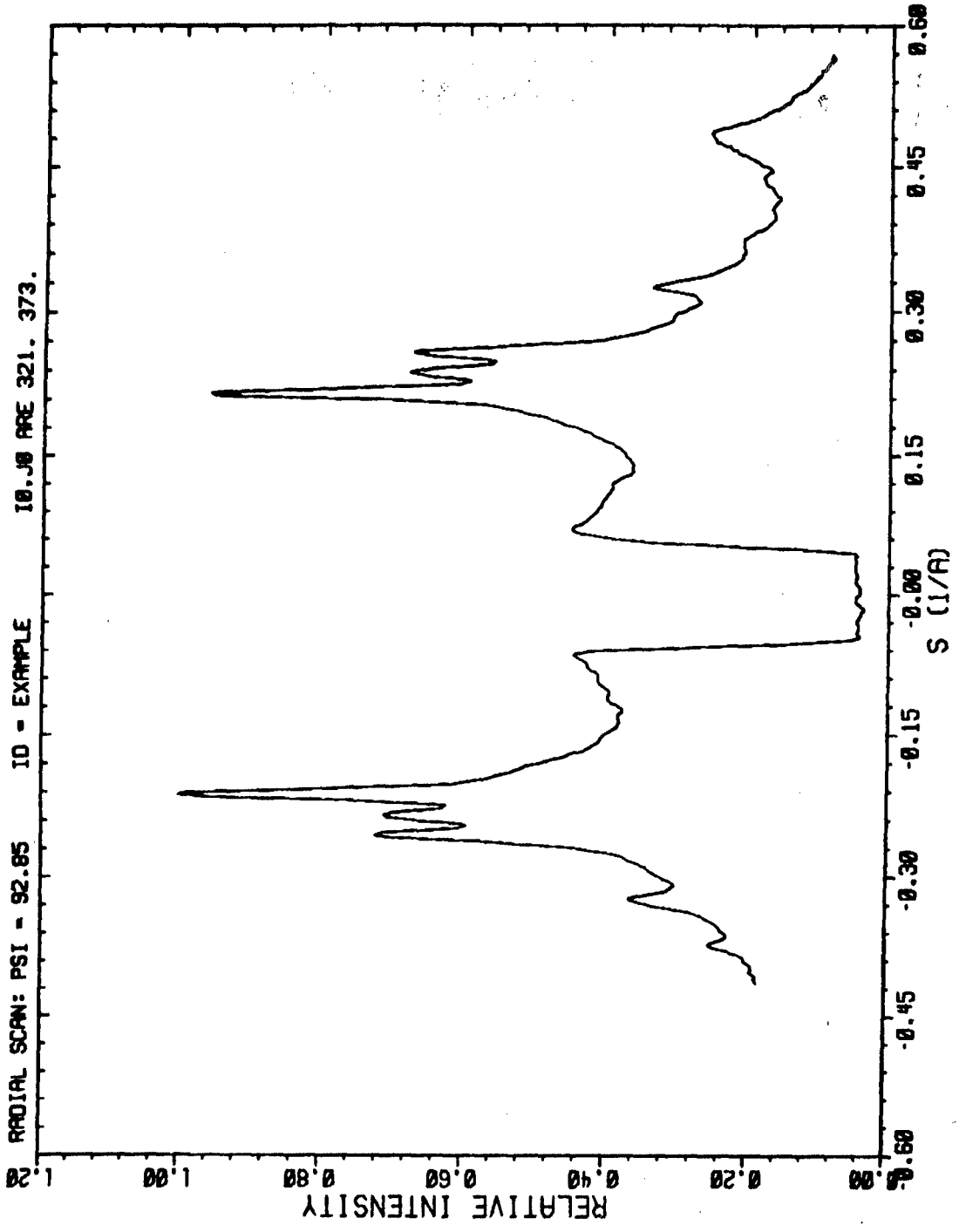

Figure 3. Radial Plot: Relative Intensity vs Scattering Vector (S).

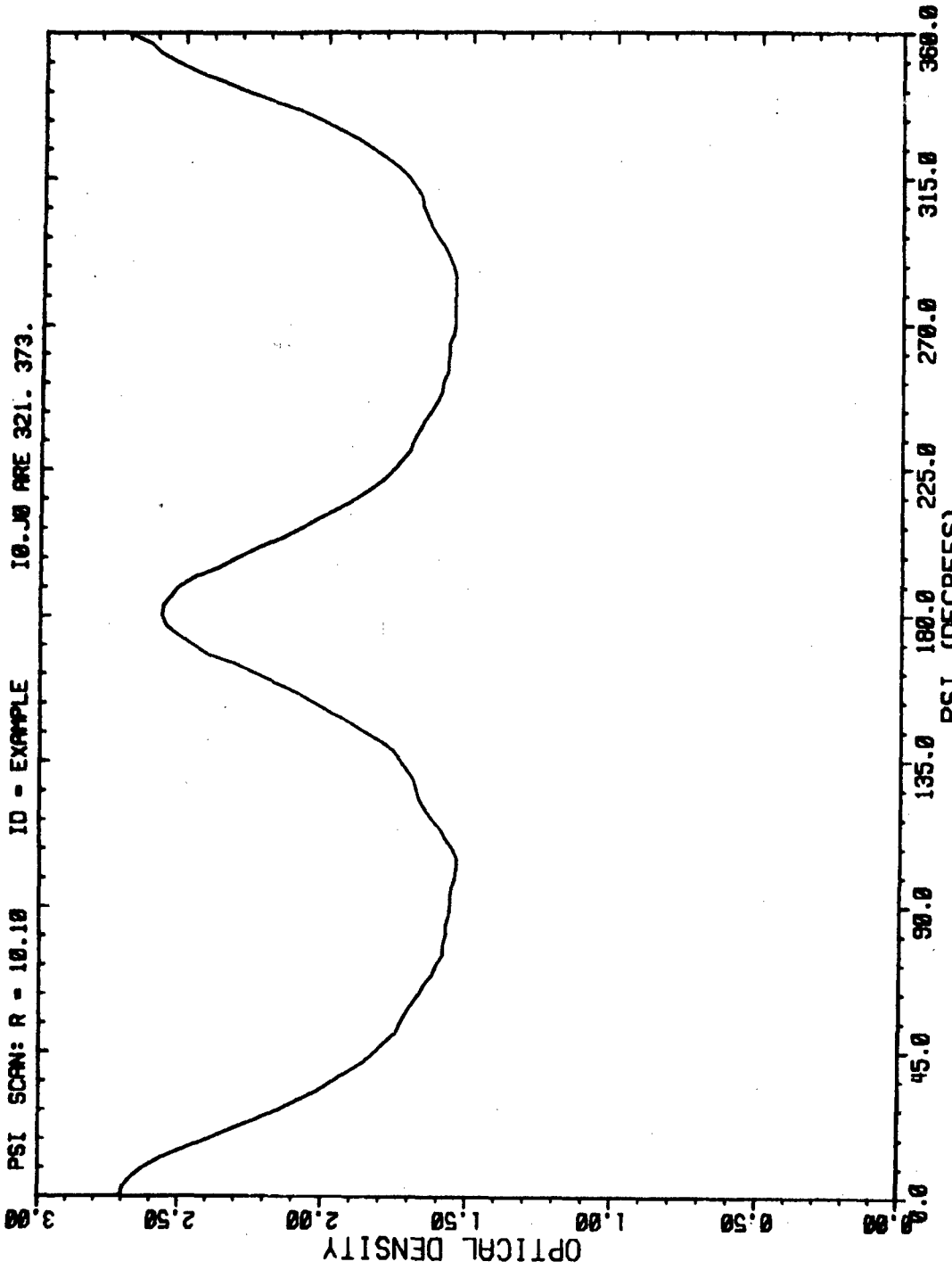

Figure 4. PSI Plot.

☆U.S. Government Printing Office: 1985 — 559-065/20711